

# p-Fluoro-N,N-dimethylaniline

|                      |                                                      |
|----------------------|------------------------------------------------------|
| Other names:         | N,N-Dimethyl-4-fluoroaniline                         |
| Inchi:               | InChI=1S/C8H10FN/c1-10(2)8-5-3-7(9)4-6-8/h3-6H,1-2H3 |
| InchiKey:            | YJEHCGOJNJUOII-UHFFFAOYSA-N                          |
| Formula:             | C8H10FN                                              |
| SMILES:              | CN(C)c1ccc(F)cc1                                     |
| Mol. weight [g/mol]: | 139.17                                               |
| CAS:                 | 403-46-3                                             |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| affp          | 924.80  | kJ/mol  | NIST Webbook   |
| basg          | 898.30  | kJ/mol  | NIST Webbook   |
| gf            | 35.23   | kJ/mol  | Joback Method  |
| hf            | -111.97 | kJ/mol  | Joback Method  |
| hfus          | 16.23   | kJ/mol  | Joback Method  |
| hvap          | 37.57   | kJ/mol  | Joback Method  |
| ie            | 7.50    | eV      | NIST Webbook   |
| log10ws       | -1.71   |         | Crippen Method |
| logp          | 1.892   |         | Crippen Method |
| mcvol         | 111.570 | ml/mol  | McGowan Method |
| pc            | 3392.03 | kPa     | Joback Method  |
| tb            | 425.81  | K       | Joback Method  |
| tc            | 622.84  | K       | Joback Method  |
| tf            | 251.92  | K       | Joback Method  |
| vc            | 0.411   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 213.88 | J/mol×K | 425.81          | Joback Method |
| cpg           | 226.68 | J/mol×K | 458.65          | Joback Method |
| cpg           | 238.77 | J/mol×K | 491.49          | Joback Method |
| cpg           | 250.18 | J/mol×K | 524.33          | Joback Method |
| cpg           | 260.93 | J/mol×K | 557.17          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 271.05 | J/mol×K | 590.01 | Joback Method |
| cpg | 280.58 | J/mol×K | 622.84 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C403463&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C403463&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>affp:</b>    | Proton affinity                                 |
| <b>basg:</b>    | Gas basicity                                    |
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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